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NONLINEAR MULTISTEP METHODS FOR INITIAL VALUE PROBLEMS

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Abstract—Some k-step kth order explicit nonlinear multistep methods (NMM) are proposed for both stiff and singular initial value problems. The algorithms are based on a local representation of the solution by the reciprocal of a polynomial. For a k-step scheme, there is need to solve a linear system of equations for the k coefficients of the inverse polynomial which are apparently global for linear differential equations.

The resultant integration schemes are stable and convergent and compare favorably with the methods of Lambert and Shaw[2], Luke, Fair and Wimp[7] and Lambert[1].

INTRODUCTION

Let us consider the initial value problem (ivp)

$$y' = f(x, y),\ y(a) = y_0; \tag{1.1}$$

$y, f \in R^m$ and $x \in [a, b]$ a finite interval on the real line. Since the new algorithms are component applicable to systems, ([1], pp. 218) of differential equations, it suffices to limit the present discussion to the scalar case, i.e. $m = 1$.

The conventional one-step scheme is given by

$$y_{n+1} = y_n + h\phi(x_n, y_n, h), \tag{1.2}$$

where $\phi(x, y; h)$ is the increment function; and the conventional linear multistep method (LMM) is described by

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f_{n+j}, \tag{1.3}$$

where α_j, β_j are real constants.

As the basis of the formulation of (1.3) is exclusively on the local representation of the theoretical solution to (1.1) by polynomials, the resultant algorithms generally perform poorly when the ivp (1.1) is stiff or its solution possesses singularities.

Lambert and Shaw [2–4, 6] and Luke, Fair, and Wimp [7] have developed non-linear algorithms to handle ivp with singularities while Lambert [5] was designed to cope with stiff systems of o.d.es. Gautschi [6] also developed non-linear multistep methods to cope with oscillatory systems.

In this paper, the author proposes an alternative approach to [2–4, 7]. Here, the theoretical solution to the ivp (1.1) is locally approximated by

$$F_k(x) = \frac{A}{\left(1 + \sum_{r=1}^{k} a_r x^r\right)} \tag{1.4}$$

where A and the coefficients a_r, $r = 1(1)k$ are real constants.

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The resultant algorithms are explicit nonlinear multistep methods which could cope with stiff ivp as well as those possessing singularities. The singularities are the poles of(1.4) and could be overstepped by adjusting the mesh-size.

The proposed algorithms are stable and their order p corresponds with the step k, (i.e. $p = k$).

2. ONE-STEP SCHEME

Consider the case when the deominator of (1.4) is linear, i.e.

$$F_1(x) = \frac{A}{(1 + a_1 x)}. \tag{2.1}$$

The theoretical solution $y(x)$ is approximated by (2.1) in the interval $[x_n, x_{n+1}]$. This implies

$$(1 + a_1 x)\, y(x) = A. \tag{2.2}$$

With the transformation $sh = x - x_0$, $x_n = x_0 + nh$ in (2.2), we readily obtain the following relationships:

$$y_0 = A, \tag{2.3a}$$

and

$$(1 + a_1) y_1 = A. \tag{2.3b}$$

Differentiating (2.1) and ensuring that it satisfies the ivp (1.1), we get

$$(1 + a_1 x)\, y'(x) = -\, a_1\, y(x) \tag{2.4}$$

which implies

$$a_1 = -\frac{h y_0'}{y_0}. \tag{2.5}$$

Eqns. (2.3) and (2.5) imply

$$y_1 = \frac{y_0^2}{(y_0 - h y_0')}. \tag{2.6}$$

In general, the one-step nonlinear integration scheme is given by

$$y_{n+1} = \frac{y_n^2}{(y_n - h y_n')}. \tag{2.7}$$

The stability of (2.7) is examined by applying it to the scalar test problem

$$y' = \lambda y,\ re\lambda < 0 \tag{2.8}$$

yielding

$$y_{n+1} = \mu(\lambda h) y_n \tag{2.9}$$

whre the stability equation is obtained as

$$\mu(\lambda h) = \frac{1}{(1 - \lambda h)} \tag{2.10}$$

which is the (0, 1) Padé approximation to $e^{\lambda h}$. This suggests not only A-stability but in fact a stronger property of L-stability.

Order and local truncation error of one-step scheme

We associate with (2.7) the nonlinear operator $N[y(x), h]$ specified by

$$N[y(x), h] = y(x+h) - y(x)^2/(y(x) - hy'(x)) \tag{2.11}$$

where $y(x)$ is some arbitrary function in $c'[a, b]$ with the constraint that $|y(x)| + |y'(x)| \neq 0$ for all $x \in [a, b]$.

The method (2.7) is said to be of *order* p if $N[y(x); h] = 0(h^{p+1})$ and the *local truncation error* T_{n+1} at x_{n+1} is given by $N[y(x_n), h]$ where $y(x_n)$ is now taken to be the theoretical solution to (1.1). It is presumed that

$$y_n = y(x_n);\; T_{n+1} = y(x_{n+1}) - y_{n+1},$$

where y_{n+1} is the numerical approximation at $x = x_{n+1}$.

By adopting the Talyor's expansion of y_{n+1} about x_n, the local truncation error is readily obtained as

$$T_{n+1} = \frac{\frac{1}{2}y_n y_n'' - y_n'^2)}{(y_n - hy_n')} h^2 + 0(h^3) \tag{2.12}$$

which suggests that (2.7) is at least of order one, i.e. $p \geq 1$ provided $y_n \neq 0$. In case $y_n = 0$, the mesh-size h can always be adjusted.

Two-step scheme

We further illustrate the discussion with the case $k = 2$ i.e. the theoretical solution $y(x)$ is locally represented in the interval $[x_n, x_{n+2}]$ by the interpolating polynomial

$$F_2(x) = \frac{A}{(1 + a_1x + a_2x^2)}. \tag{2.13}$$

By constraining (2.13) to approximate the theoretical solution at the points: x_0, x_1 and x_2, we have (with the translation earlier introduced):

$$\begin{aligned} y_0 &= A, \\ (1 + a_1 + a_2)y_1 &= A, \\ (1 + 2a_1 + 4a_2)y_2 &= A. \end{aligned} \tag{2.14}$$

If (2.13) satisfies the ivp (1.1) at $x = x_0$ and $x = x_1$, we also have

$$hy_0' + a_1y_0 = 0, \tag{2.15a}$$

and

$$(1 + a_1 + a_2)hy_1' + (a_1 + 2a_2)y_1 = 0. \tag{2.15b}$$

Solve (2.15) for a_1 and a_2 and get

$$a_1 = -\frac{hy_0'}{y_0}, \tag{2.16}$$

and

$$a_2 = \frac{\left\{\dfrac{hy_0'}{y_0}(hy_1' + y_1) - hy_1'\right\}}{(hy_1' + 2y_1)}. \tag{2.17}$$

From equation (2.14) we derive the 2-step NMM

$$y_2 = \frac{(1+a_1+a_2)^2}{(1+2a_2+4a_2)}\frac{y_1^2}{y_0}. \tag{2.18}$$

In general,

$$a_1 = -\frac{hy'_n}{y_n}, \tag{2.19}$$

$$a_2 = \frac{\left\{\frac{hy'_n}{y_n}(hy'_{n+1}+y_{n+1}) - hy'_{n+1}\right\}}{(hy'_{n+1}+2y_{n+1})}, \tag{2.20}$$

$$y_{n+2} = \frac{(1+a_1+a_2)^2}{(1+2a_1+4a_2)}\frac{y_{n+1}^2}{y_n}. \tag{2.21}$$

The application of (2.21) to (2.8) yields

$$a_1 = -\lambda h, \tag{2.22}$$

$$a_2 = \frac{(\lambda h)^2}{(\lambda h+2)}, \tag{2.23}$$

$$y_{n+2} = \mu_2(\lambda h)\frac{y_{n+1}^2}{y_n}, \tag{2.24}$$

with the stability equation $\mu_2(\lambda h)$ satisfying:

$$\lim_{\lambda h \to -\infty} \mu_2(\lambda h) = 0 \tag{2.25}$$

which suggests L-stability of the 2-step NMM.

Generalization of the nonlinear methods

We now consider the case when the degree of the inverse polynomial is arbitrary.

Differentiating (1.4) with respect to x implies

$$\sum_{j=1}^{k} (y'_i x_i^j + j y_i x_i^{j-1}) a_j = hy'_i, \tag{2.26}$$

for $i = 0(1)k-1$. With $x = x_0 + ih$ and $s = x - x_0$, and replacing y'_i by hy'_i, equation (2.26) gives

$$\sum_{j=1}^{k} (hi^j y'_i + j i^{j-1} y_i) a_j = -hy'_i \tag{2.27}$$

for $i = 0(1)\, k-1$.

This can be compactly expressed as

$$Ra = b, \tag{2.28}$$

where

$$R_{ij} = hi^j y'_i + j i^{j-1} y_i\,;\ (i, j = 1(1)k) \tag{2.29}$$

and

$$b_i = -hy'_i \quad i = 0(1)k-1. \tag{2.30}$$

The system (2.28)–(2.30) has a unique solution provided

$$\Delta = \det(R) \neq 0. \tag{2.31}$$

If (2.31) is violated, the presence of a singularity is indicated. In this event one can always adjust the stepsize to overstep this singularity.

By further constraining the interpolating function (1.4) to coincide with the theoretical solution at the meshpoints x_j, $j = 0(1)k$, we readily obtain the integration formula

$$y_{n+k} = \frac{y_n}{(1+\sum_{r=1}^{k} k^r a_r)}, \tag{2.32}$$

with the coefficients a_r, $r = 1(1)k$ obtained from equation (2.28).

3. NUMERICAL EXPERIMENTS

All the numerical experiments were performed in double precision on Prime 750 situated at the University of Benin Computer Centre.

We first consider the well known scalar initial value problem

$$y' = 1 + y^2,\ y(0) = 1 \tag{3.1}$$

whose theoretical solution is $y(x) = \tan(x + \pi/4)$. The new schemes were applied to problem (3.1) for $k = 1(1)7$.

Besides, the same problem was solved with

(a) Trapezoidal scheme, i.e.

$$y_{n+1} = y_n + \frac{h}{2}(y'_n + y'_{n+1}) \tag{3.2}$$

(b) Taylors series method of order four, i.e.

$$y_{n+1} = y_n + \sum_{r=1}^{4} \frac{h^r}{r!} y_n^{(r)} \tag{3.3}$$

Table 1(a). Coefficients of inverse polynomial at $x = 0$

k	a_1	a_2	a_3	a_4	a_5	a_6	a_7
1	−0.0999999						
2	−0.0999999	0.0045456					
3	−0.0999999	0.0049351	−0.0002638				
4	−0.0999999	0.0049872	−0.0003168	0.0000133			
5	−0.0999999	0.0049969	−0.0003289	0.1834179	−0.000000		
6	−0.999999	0.0049991	−0.0003320	0.0000199	−0.000001	0.0000000	
7	−0.0999999	0.0049966	−0.0003284	0.0000180	−0.000000	−0.0000000	−0.00000000

Table 1(b). Coefficients of inverse polynomial at $x = 0.75$

k	a_1	a_2	a_3	a_4	a_5	a_6	a_7
1	−0.7420385						
2	−0.3705786	0.0022342					
3	−0.2761732	0.0025595	−0.0002347				
4	−0.2204449	0.0026451	−0.0002116	0.0000028			
5	−0.1850848	0.0027131	−0.0001920	0.0000044	−0.0000001		
6	−0.1228269	−0.6543635	−1.1180598	−0.6113667	0.1339063	−0.0100917	
7	−0.1435254	0.0029212	−0.0001903	0.0000096	−0.000005	−0.0000000	−0.0000000

Table 2. $y' = 1 + y^2$, $y(0) = 1$, theoretical solution $y(x) = \tan(x + \pi/4)$. Errors in nonlinear multistep methods

X	Theoretical Solution	$k = 1$	$k = 2$	$k = 3$	$k = 4$	$k = 5$	$k = 6$	$k = 7$
0.00	1.000,000,000	-	-	-	-	-	-	-
0.10	1.223,048,880	1.22816(−2)	−8.27741(−4)	-	-	-	-	-
0.20	1.508,497,647	2.91873(−2)	−1.89419(−3)	2.29807(−4)	−5.95328(−5)	-	-	-
0.30	1.895,765,123	5.57996(−2)	−3.51966(−4)	5.50660(−4)	−5.43415(−5)	2.30964(−5)	3.68323(−3)	-
0.40	2.464,962,757	1.04486(−1)	−6.47338(−3)	6.72580(−4)	−1.68543(−4)	2.40806(−5)	1.45228(−1)	−1.67127(−4)
0.50	3.408,223,442	2.13434(−1)	−1.31241(−2)	1.75434(−3)	−2.23773(−4)	7.23361(−3)	−4.55561(0)	−3.12818(−5)
0.60	5.331,855,223	5.56258(−1)	−3.40542(−2)	4.20614(−3)	−7.54129(−4)	1.27200(−4)	−5.25156(0)	−2.88453(−4)
0.65	7.340,436,575	1.10611(0)	−6.63368(−2)	8.37905(−3)	−1.50951(−3)	2.33836(−4)	−7.37683(0)	−9.87554(−4)
0.70	11.681,373,800	3.09171(0)	−1.76210(−1)	2.01607(−2)	−3.32208(−3)	7.84943(−3)	−1.18516(1)	−1.79499(−3)
0.75	28.238,252,850	2.90303(1)	−1.07376(0)	1.18085(−1)	−1.89317(−2)	4.90205(−3)	−2.82323(1)	−7.87842(−3)

Index $a(-b) = a \cdot 10^{-b}$

Table 3. Errors in numerical solution

X	Trapezoidal scheme (3.2)	Fatunla $L = 2$	Lambert and Shaw[6] order 2, equation (3.4)	Taylor's series order, 4, equation (3.3)	Fatunla $K = 4$	Luke, Fair[1] and Wimp $K = 2$, order 4, equation (3.6)	Lambert and Shaw[6] order 4, equation (3.5)
0.00	–	–	–	–	–	–	–
0.10	5(−4)	−8(−4)	1(−4)	3(−6)	–	1(−5)	8(−8)
0.20	2(−3)	−1(−3)	3(−4)	1(−5)	6(−5)	2(−5)	2(−7)
0.30	4(−3)	−3(−3)	6(−4)	5(−5)	5(−5)	3(−5)	4(−7)
0.40	1(−2)	−6(−3)	1(−3)	2(−4)	2(−4)	3(−5)	7(−7)
0.50	3(−2)	−1(−2)	3(−3)	7(−4)	2(−4)	7(−5)	1(−6)
0.60	2(−1)	−3(−2)	7(−3)	5(−3)	7(−4)	2(−4)	4(−6)
0.65	5(−1)	−6(−2)	1(−2)	2(−2)	1(−3)	4(−3)	8(−6)
0.70	3.4(0)	−2(−1)	4(−2)	1(−1)	3(−3)	1(−2)	2(−5)
0.75	–	−1(0)	3(−1)	3(0)	1(−2)	1(−1)	1(−4)

Index $a(-b) = a.10^{-b}$

(c) Lambert and Shaw nonlinear schemes [3], i.e.

(i)
$$y_{n+1} = y_n + h^2 \frac{y'_n y'_{n+1}}{y_{n+1} - y_n}, \tag{3.4}$$

(ii)
$$y_{n+1} = y_n + \sum_{r=1}^{3} \frac{h^r}{r!} y_n^{(r)} + \frac{h^4}{6} \frac{y_n^{(3)} y_n^{(4)}}{(4y_n^{(3)} - hy_n^{(4)})} (4) \tag{3.5}$$

(d) Luke, Fair and Wimp rational interpolation scheme [7] for the case $m = 1$ and $n = 2$, *i.e.*

$$y_{n+2} = \frac{y_n^2(3y_{n+1} + hy'_{n+1}) + y_{n+1}^2(2hy'_n - 3y_n)}{y_n(4y_n - 5y_{n+1} + hy'_{n+1}) + y_{n+1}(y_{n+1} + 2hy'_n) - 2h^2 y'_n y'_{n+1}}. \tag{3.6}$$

All the numerical solutions were generated with a uniform meshsize $h = 0.05$ in the interval $0 \le x \le 0.75$

Table 1 gives the coefficients of the inverse polynomial at $x = 0$ and $x = 0.75$ while Table 2 gives details of the numerical solution to problem (3.1) for $k = 1(1)7$. Table 3 confirms the poor performance of the numerical integration schemes which are based on polynomial interpolation on ivp with singularities i.e. formulas (3.2) and (3.3).

We further consider the stiff ivp

$$y' = -200(y - E(x)) + E'(x), \; y(0) = 10 \tag{3.7}$$

where

$$E(x) = 10 - (10 + x)\, e^{-x} \tag{3.8}$$

in the interval of $0 < x \le 100$ using $k = 1$ with uniform mesh sizes $h = 0.001$. and $h = 0.005$. The theoretical solution is $y(x) = E(x) + 10\, e^{-200x}$.

This same problem has also been solved by the following schemes:

(a) Fourth order Runge–Kutta scheme (Rk4)
(b) Adams fourth order predictor corrector scheme (ADAM)
(c) Treanor's scheme (TRN)
(d) Trapezoidal scheme (TRAP)
(e) Trapezoidal scheme with extrapolation (EX-TRAP)
(f) Liniger and Willoughby (LW1, LW2)
(g) Fatunla [2].

Table 4.

Method	h	$x = 0.4$	$x = 10$
RX 4	0.01	1.0(−5)	2.0(−9)
ADAM	0.005	3.0(−9)	2.0(−9)
TRN	0.2[a]	6.7(−8)	1.0(−9)
TRAP	0.2	1.8(−2)	4.3(−8)
EX-TRAP	0.2	1.4(−4)	1.0(−8)
LW1	0.2	1.1(−3)	5.0(−8)
LW2	0.2	1.8(−3)	9.0(−8)
Fatunla [8]	0.2	1.4(−6)	8.3(−8)
Formula (2.7)	0.005	4.0(−4)	1.0(−8)
Formula (2.7)	0.001	8.1(−5)	2.0(−9)

Index: *a* automatic step size.

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